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Total No. Pages - iii and 37

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ENGINEERING ESTIMATES OF FLOW
LENGTHS ASSOCIATED WITH THE
COMBUSTION OF HYDROGEN-AIR
MIXTURES DURING A LAUNCH
TRAJECTORY

By: P. A. Libby - H. S. Pergament
P. Taub

TECHNICAL REPORT No. 330

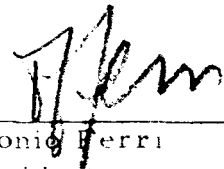
Prepared for

George C. Marshall Space Flight Center
Huntsville, Alabama
Contract No. NAS8 - 2686

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December 28, 1962

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SYMBOLS

k_{fi}	forward reaction rate for reaction i
M_e	Mach number at edge of boundary layer
p	static pressure
T	static temperature
u	velocity
γ	ratio of specific heats
τ_{ID}	ignition delay time
τ_R	reaction time
Y	mass fraction

SUBSCRIPTS

e	value at edge of boundary layer
i	initial value
m	value at position of maximum temperature in the boundary layer
w	wall value
1	refers to species 1 (C_2)
2	" 2 (H_2)
3	" 3 (H_2O)
5	" 5 (O)
6	" 6 (H)
7	" 7 (OH)

ENGINEERING ESTIMATES OF FLOW LENGTHS ASSOCIATED WITH THE
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I. INTRODUCTION.

During the atmospheric exit of a launch vehicle utilizing hydrogen in its upper stages, it appears that gaseous or liquid hydrogen is sometimes dumped overboard into the airstream. If the flow conditions are such as to lead to no significant chemical reactions while the resulting hydrogen-air mixture is in the proximity of the launch vehicle, this dumping will be of little importance. On the contrary if combustion does occur, there can occur significant alteration of the heat transfer to surface of the vehicle and of the aerodynamic forces and moments applied to the vehicle.

As an initial step in a program of analysis of the phenomena arising when hydrogen is ejected overboard from a launch vehicle, the flow lengths associated with both the induction (or ignition delay) period and heat release (or reaction) period of the hydrogen-air reaction have been computed for a typical exit trajectory. On the basis of research connected with the kinetics of the hydrogen-oxygen system and with the supersonic combustion of hydrogen, the main features

of the reaction history of this combustion are understood. There exists two phases; the first, so-called induction period⁽¹⁾ involves major alterations in composition, the formation of water and of intermediate species, but no significant heat release, i. e. no temperature rise. During the second period, the concentrations of the intermediates decay and heat is released. The times associated with both periods are readily estimated for a given pressure and initial temperature. It is therefore possible to apply such estimates to determine the flow lengths associated with the induction and heat release periods and thus to estimate under what flow conditions combustion in the vicinity of the launch vehicle can be expected. Such estimates do not include delays due to vaporization of liquid fuel and to mixing of the hydrogen with the air⁽²⁾; detailed studies of these processes are required to obtain more accurate estimates of the phenomena.

During an exit trajectory there are two counteracting effects influencing the induction time; as the launch vehicle accelerates, the static pressure near the vehicle decreases, tending to increase induction times, while the maximum

(1) This period is defined here as the time required for the temperature to increase an amount equal to 5% of the total temperature rise to equilibrium.

(2) The results obtained from this analysis are thus conservative.

static temperature, for example, that in the boundary layer and behind strong shock waves, increases tending to decrease such times. Accordingly, it might be expected that the estimated flow lengths may have a minimum; this will be found to be the case.

In this report the current information on the kinetics of the hydrogen-air system is reviewed first. Then, for a typical exit trajectory the flow lengths associated with the induction and reaction periods and a critical altitude range for combustion in the neighborhood of the launch vehicle are presented.

The authors are pleased to acknowledge that Dr. Antonio Ferri suggested this study.

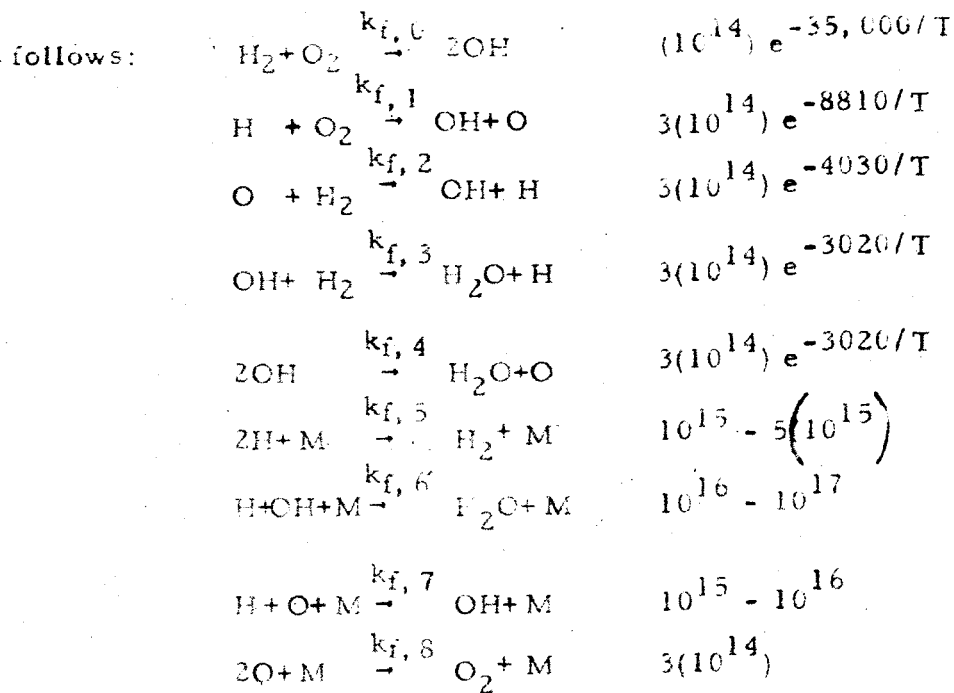
II. THE MECHANISMS AND KINETICS OF THE HYDROGEN-AIR SYSTEM

For the temperature range below 2300°K , it appears that the nitrogen in air can be treated as an inert diluent with respect to the hydrogen-air reaction. Accordingly, the extensive research devoted to the hydrogen-oxygen system can be employed in the study of the mechanisms and kinetics of the combustion of hydrogen in air. Recently, there has been considerable attention given to the use of hydrogen as a fuel in an advanced air-breathing engine. References 1-5 have studied inter alia flows involving reacting hydrogen-air mixtures with finite rate chemistry. The actual rate constants used in these analyses differ in some cases by an order of magnitude in the temperature range from 1000 to 3000°K ; these differences reflect existing ignorance in kinetic information. On the other hand, the mechanisms, i.e., the reaction steps, are generally based on the research of Duff and co-workers (References 6-8) and are thus generally the same in all studies.

As will be seen below, the mechanisms of the hydrogen-oxygen reaction are so complex that they cannot be verified in detail; experiments can, in general, only confirm or reject the validity of the total ensemble of reaction steps and reaction rates. The predictions based on the ensemble described herein and employed in the analyses listed above are in accord with shock tube data, e.g., of Schott et al (References 7 and 8), with the experiments of Nicholls (Reference 9), with the nozzle experiments of Lezberg and Lancashire

(Reference 10)*, and with experiments on supersonic diffusion flames (Reference 5). Accordingly, over a range of initial temperatures, i.e., prior to heat release, of from 1000° to 2000°K and over the pressure range from 10^{-1} to 4 atmospheres the reaction steps and rates employed here can be considered to yield consistent predictions, in accord with experiment, in an overall sense. No experimental data appears to be available outside this range of conditions.

If nitrogen is treated as an inert diluent, the mechanisms and rates for reactions proceeding to the right involved in hydrogen-air combustion are as follows:



* Cf., Reference 5 for the comparison between theory and experiment.

The temperatures are in $^{\circ}\text{K}$ and the units for k_f are $(\text{mole/cc})^{-1} \text{sec}^{-1}$ for second order reactions and $(\text{mole/cc})^{-2} \text{sec}^{-1}$ for third order reactions; the symbol M denotes any third body. The first reaction step, i.e., related to $k_{f,0}$ involves a relatively high activation energy and is thus usually neglected in the temperature range of aeronautical interest. For several of the three-body reactions, a range of values for the rate constants has been shown; these were presented by Duff and co-workers as bracketing the range of estimated values. Finally, it is noted that these mechanisms should not be employed below roughly 900°K because the classical work on explosions, (cf. e.g., Reference 11) indicates that hydrogen-oxygen mixtures are stable at all pressures provided a temperature of roughly this value is not exceeded. If the reaction steps given above were formally applied at low temperatures, it is quite possible that a numerical solution for a reaction history would yield a large but finite reaction time in disagreement with experiment.

In Reference 1 (cf., Reference 5), the reaction steps corresponding to $k_{f,i}$, $i = 1, 2, \dots, 8$ were applied to flows with constant pressure and constant energy. A uniform mixture of hydrogen and air at an initial temperature T_i and a constant pressure p was assumed to exist at time zero; the reaction history of this mixture was studied by numerical integration of the species conservation equations. The results of this analysis indicated that the hydrogen-oxygen reaction consists of two phases; during the initial, so-called induction (or ignition delay) phase, significant changes in composition take place with little change in temperature. Indeed, the composition at the end of this phase is close to equilibrium insofar as major constituents are concerned, but the

concentrations of the intermediates, O, H and OH, although present to the extent of one percent or less on a mass fraction basis, far exceed their equilibrium values. This behavior for a number of pressures and initial temperatures for an equivalence ratio of unity is shown in Figure 1, which has been taken from Reference 5. The uniformity of the temperature during this phase is accounted for roughly by the absorption in dissociation of molecular hydrogen of the heat released by the formation of water. During the second phase, termed in Reference 5 the heat release phase, the excess of intermediates decay to their equilibrium values, the major constituents adjust somewhat their concentrations and the temperature increases. These effects can also be noted in Figure 1 where R. R. #2 refers to intermediate values of the reaction rates for the recombination reaction; it is believed that these rate constants represent the best available data and should give accurate results.

The induction phase is controlled by the two-body reactions while the heat release phase is governed by the three-body reactions. As a consequence of this change in the dominant reactions in each phase, the pressure dependence of the times associated with each phase is different, the induction time varying as p^{-1} and the heat release time varying as $p^{-1.7}$. Under conditions of low pressure and high initial temperature, the induction time becomes negligible compared to the heat release time; for example, at $p = 1$ atmosphere, $T_i = 1500^\circ \text{K}$,

$$\tau_R \approx 10\tau_{ID}$$

By use of the analysis presented in Reference 1 both the ignition delay and reaction times have been computed for a wide range of initial temperatures, T_i and pressures. From the results of the calculations it was possible to obtain the following empirical correlations:*

$$\tau_{ID} p \approx 8 \times 10^{-3} e^{9600/T_i} \quad (1)$$

$$\tau_{R} p^{1.7} \approx 105 e^{-1.12 \times 10^{-3} T_i} \quad (2)$$

where the times are in μ sec., T_i in $^{\circ}$ K, and p in atmospheres.

Again, it should be noted that the above equations have been determined for the case of a uniform mixture of reactants and implicitly assumes that the mixing length is negligible compared to the chemical reaction length.

Note from equations (1) and (2) that both times decrease with increasing pressure, that τ_{ID} is extremely sensitive to temperature, decreasing sharply as T_i increases, while τ_R is a weaker function of the initial temperature, decreasing slightly as T_i increases. These correlations therefore imply that under conditions of low pressure and high temperature such as may occur during an existing trajectory, the induction period may be of short duration while the heat release phase might be long.

* A similar expression for the induction time was presented in Reference 5; the one presented here is based on additional numerical results and is considered somewhat more accurate.

III. REPRESENTATIVE INJECTION MODES FOR HYDROGEN DUMPING

Consider now the application of the previous discussion to the engineering problem of estimating the flow lengths associated with combustion of hydrogen when ejected overboard from a launch vehicle. As discussed in the Introduction the description of the actual phenomena which may be involved in such cases will be complicated and will depend on the mode of ejection, the airstream conditions and the characteristics of the dumped hydrogen. Vaporization, mixing and flow interaction effects will alter the distances from the ejection point on the launch vehicle to the downstream point where combustion takes place. Conservative flow lengths can be computed if the induction and reaction times given by Equations (1) and (2) are multiplied by a representative flow velocity. The previously cited effects will in general lead to larger flow lengths. However, these estimates can be employed to make judgments as to the injection modes leading to the smallest probability of combustion arising in a given exit trajectory.

In the present report the representative modes of dumping are examined qualitatively in order to establish approximate conditions of velocity, pressure and temperature in the zone of possible combustion. These modes are shown schematically in Figure 2 and are discussed below.

If the hydrogen is injected through a port in the skin of the vehicle as shown schematically in Figure 2a, there will, in general occur a complex flow involving a strong shock wave, boundary layer separation and reattachment, and rapid mixing between the hydrogen jet and the air stream.* For the purposes of

* The flow associated with injection of this type is also of interest in connection with thrust vectoring by injection. Ref. 12 provides a recent review thereof.

the present report the induction and heat release times are computed by assuming that the pressure and temperature are those behind a normal shock and that the velocity is associated with an isentropic expansion from conditions behind a normal shock to free stream static pressure. Such velocities would occur in the neighborhood of the jet as well as downstream of the point of injection.

Consider next the injection mode shown schematically in Figure 2b; the hydrogen is injected parallel to the external stream from a tube which causes a strong shock wave. In this case the pressure in the mixing region is close to that in the external stream but the boundary layer on the tube can result in static temperatures within the mixing region in excess of those prevailing in the external stream. The velocities at the outer edge of the mixing region can be represented by those obtained by expanding isentropically from conditions behind a normal shock to ambient pressure.

A similar situation arises in connection with slot injection as shown in Figure 2(c). However, in this case, the velocity at the edge of the mixing region is that of the external stream since no strong shock should exist. Because the static temperatures in the boundary layer either on the mixing tube or on the splitter plate may be considered, from a conservative point of view, to be representative of those in the boundary layer in a high speed flow, it is of interest to estimate the static temperature distributions therein. Within the approximation of Prandtl number equal to unity for both laminar and turbulent

flow, the Crocco relation can be applied to relate the temperature and velocity distributions. The static temperature and Mach number in the external stream, and the wall temperature are parameters. If the gas is considered as calorically and thermally perfect, as is justified for estimates in the supersonic and low hypersonic flight regions, there is obtained,

$$T/T_e = (T_w/T_e) + (u/u_e) \left[1 + (\gamma - 1) (M_e^2/2) - (T_w/T_e) \right] - (\gamma - 1) (M_e^2/2) (u/u_e)^2 \quad (3)$$

It is easy to show that the maximum static temperature within the layer is

$$T_m/T_e = (T_w/T_e) + \left[1 + (\gamma - 1) (M_e^2/2) - (T_w/T_e) \right]^2 / \left[(\gamma - 1) 2M_e^2 \right] \quad (4)$$

and that the velocity at which the temperature reaches a maximum is

$$u/u_e = \left[1 + (\gamma - 1) (M_e^2/2) - T_w/T_e \right] / (\gamma - 1) M_e^2 \quad (5)$$

For both tube and slot injection the maximum temperature in the boundary layer is used to compute the ignition delay and reaction times; the velocity at the point of peak temperature is then used to calculate the corresponding lengths.

IV. ESTIMATES OF FLOW LENGTHS FOR COMBUSTION

The launch trajectory used for the present calculations is shown in Figure 3 and, for convenience, the variation of ambient pressure with altitude is given in Figure 4. Figures 5, 6, and 7 show both the ignition delay length and the length required for a constant pressure reaction to come to equilibrium (ignition delay length plus reaction length) for the three injection schemes discussed in the previous section. It can be seen that combustion takes place in the smallest distance for the case of normal injection. This is due to the relatively high temperature and pressure existing behind the normal shock. Considerably larger ignition delay lengths are indicated when hydrogen is injected either through a tube or a slot. However, due to the low ambient pressure the reaction lengths are several orders of magnitude greater over most of the trajectory. Due to the counteracting effects of pressure and temperature, as mentioned in the Introduction, a minimum in flow length curves is observed. It would appear that from these results both tube and slot injection of hydrogen are equally favorable with regard to combustion lengths.

It should be noted that, in Figures 6 and 7, the ignition delay curves for wall temperatures of 2000°R and 3000°R cross each other. This is due to the higher velocities at the point of maximum temperature in the boundary layer, over a part of the trajectory, for the 3000°R wall temperature.

V. CONCLUSIONS

From the results of the present investigation it can be concluded that dumping hydrogen either through a slot or tube parallel to the free stream gives considerably longer combustion lengths than for normal injection. There results a critical altitude from 125 to 175 kilo feet depending on the mode of injection.

Some general comments regarding the hydrogen dumping problem can also be made as a result of this study. In devising an injection scheme advantage should be taken of the low ambient pressure over most of the trajectory (Fig. 4); that is, the hydrogen should be injected in such a way as to cause the least disturbance (and consequent pressure rise) to the free stream. In addition the injection station should be located at a position where the effects of any shock caused by the body are minimal. Since low initial temperatures are also favorable it seems that, keeping the surface temperature of the vehicle as low as possible could be an effective means of reducing the peak temperature in the boundary layer (for the range of flight conditions considered here).

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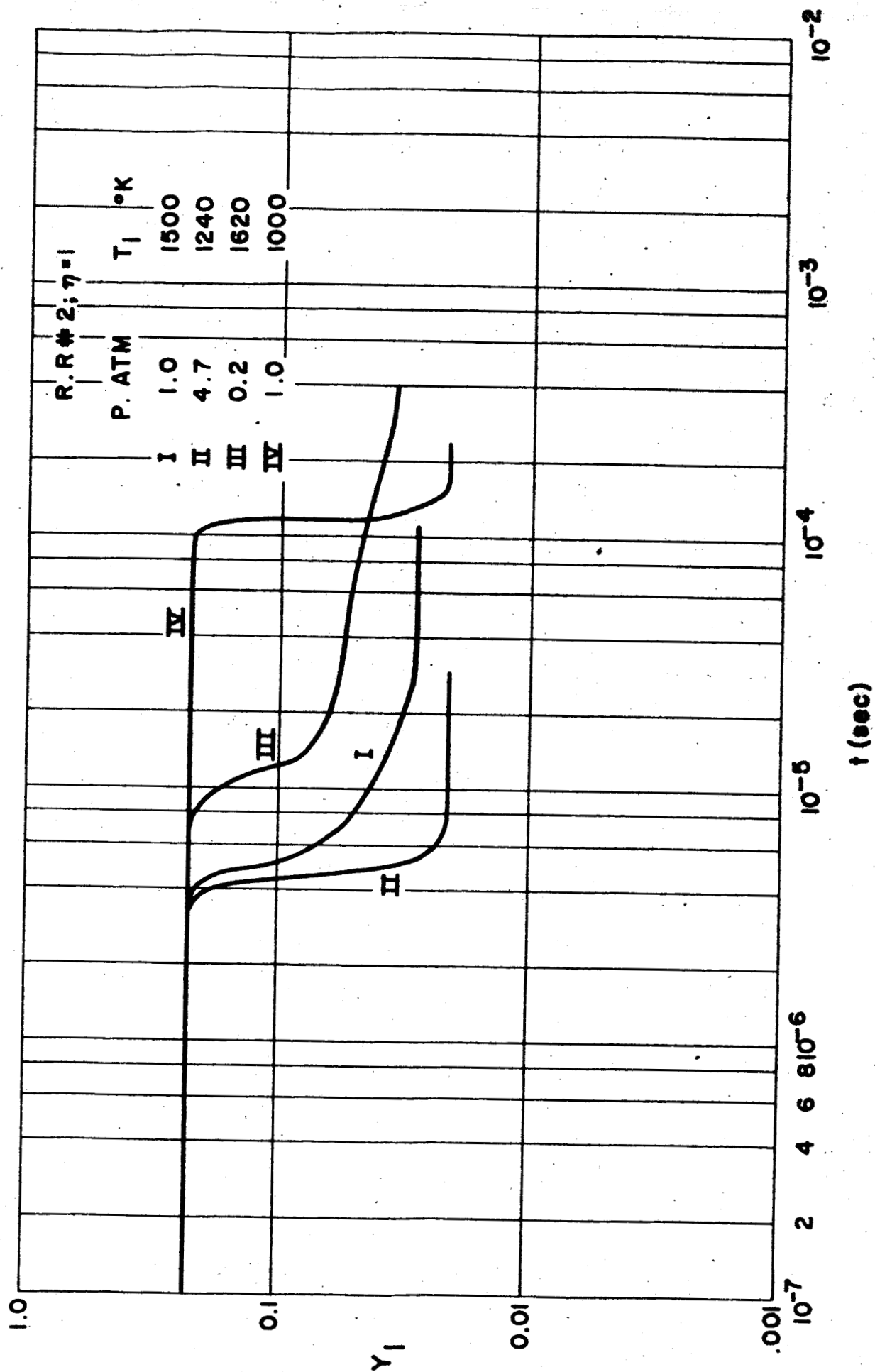


FIG. 1a Composition-Time Histories of Hydrogen-Air Mixtures at Constant Pressure.

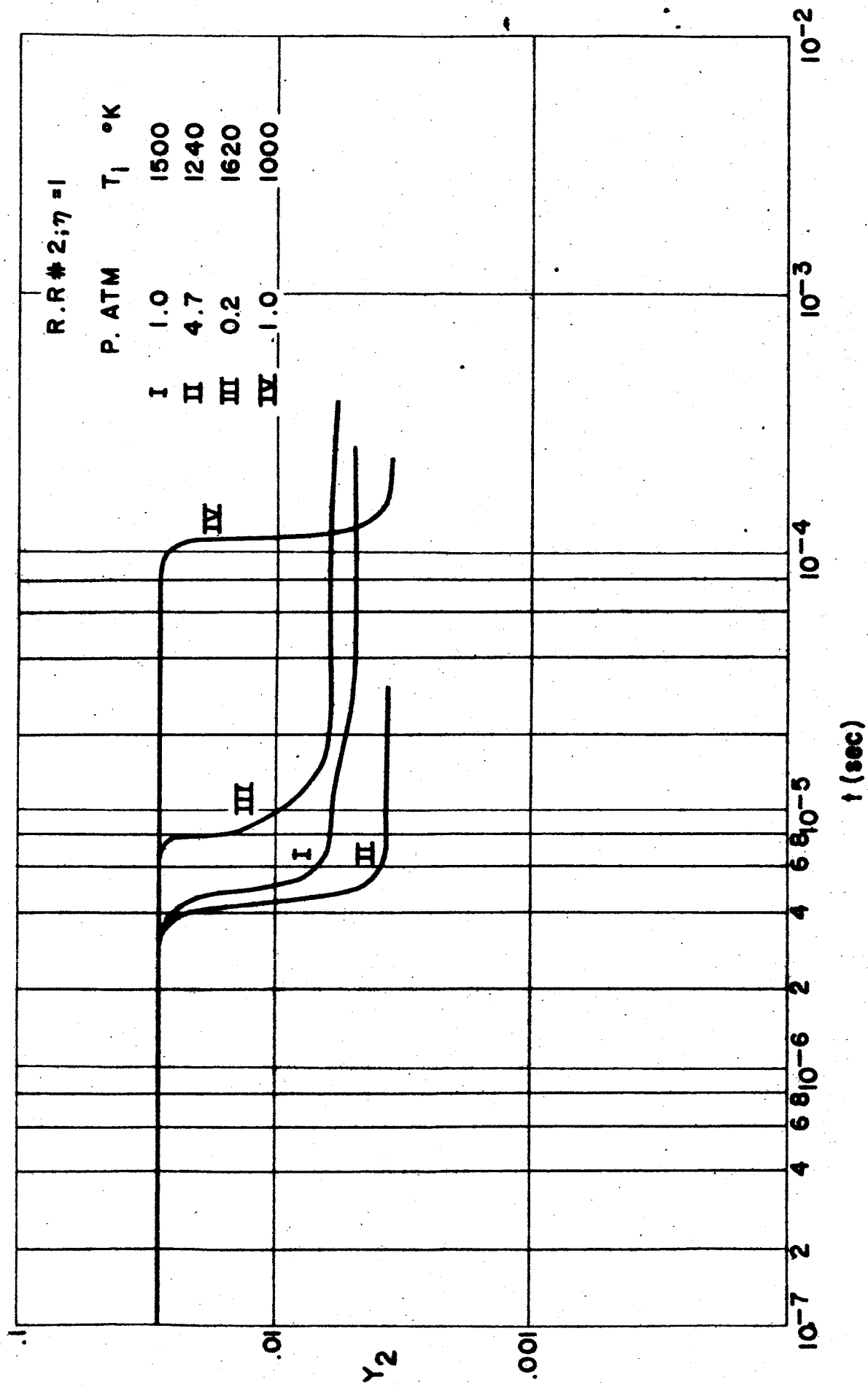


FIG. 14 Composition-Time Histories of Hydrogen-Air Mixtures at Constant Pressure, H_2 .

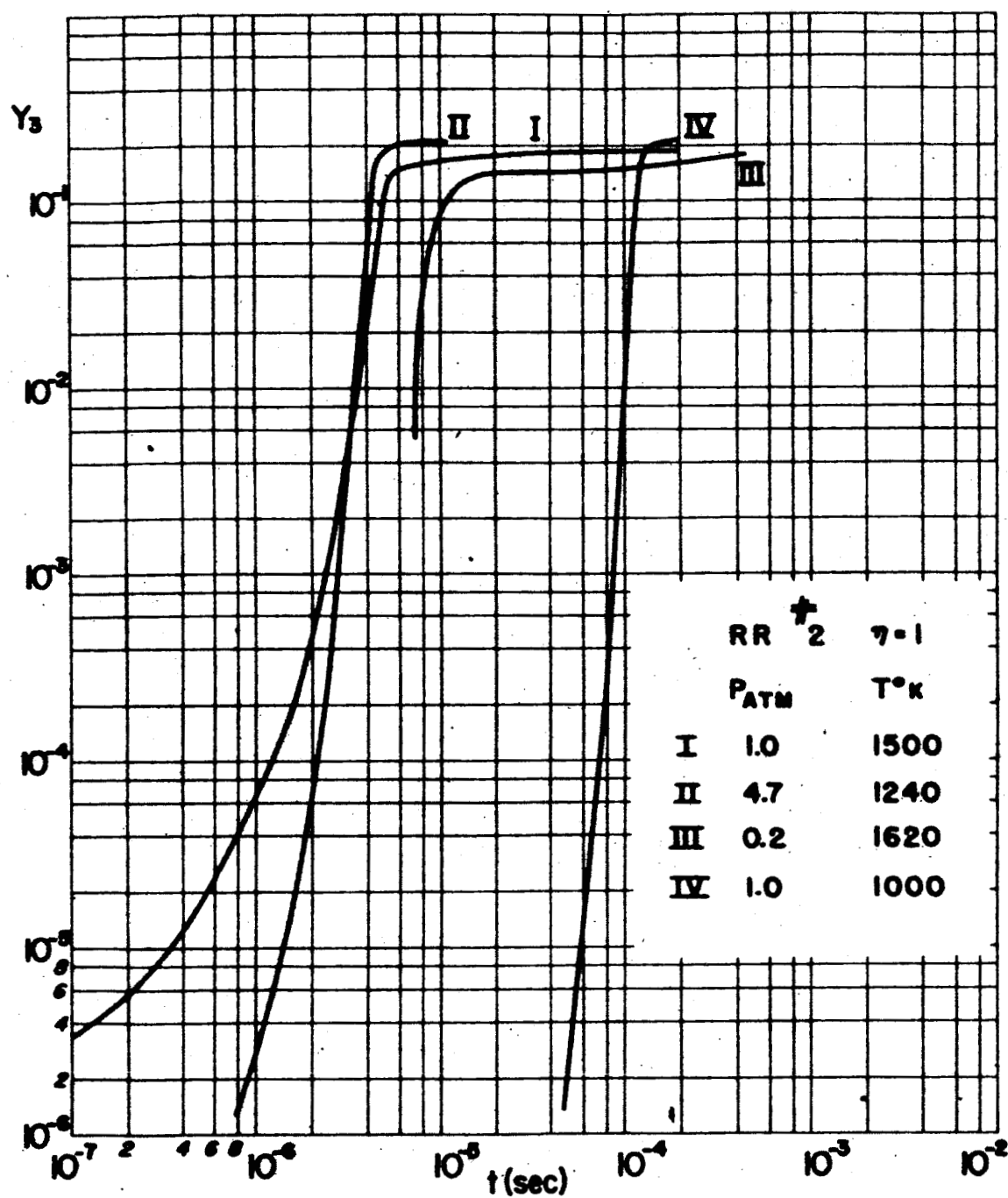


FIG. 1c Composition-Time Histories of Hydrogen-Air Mixtures at Constant Pressure.

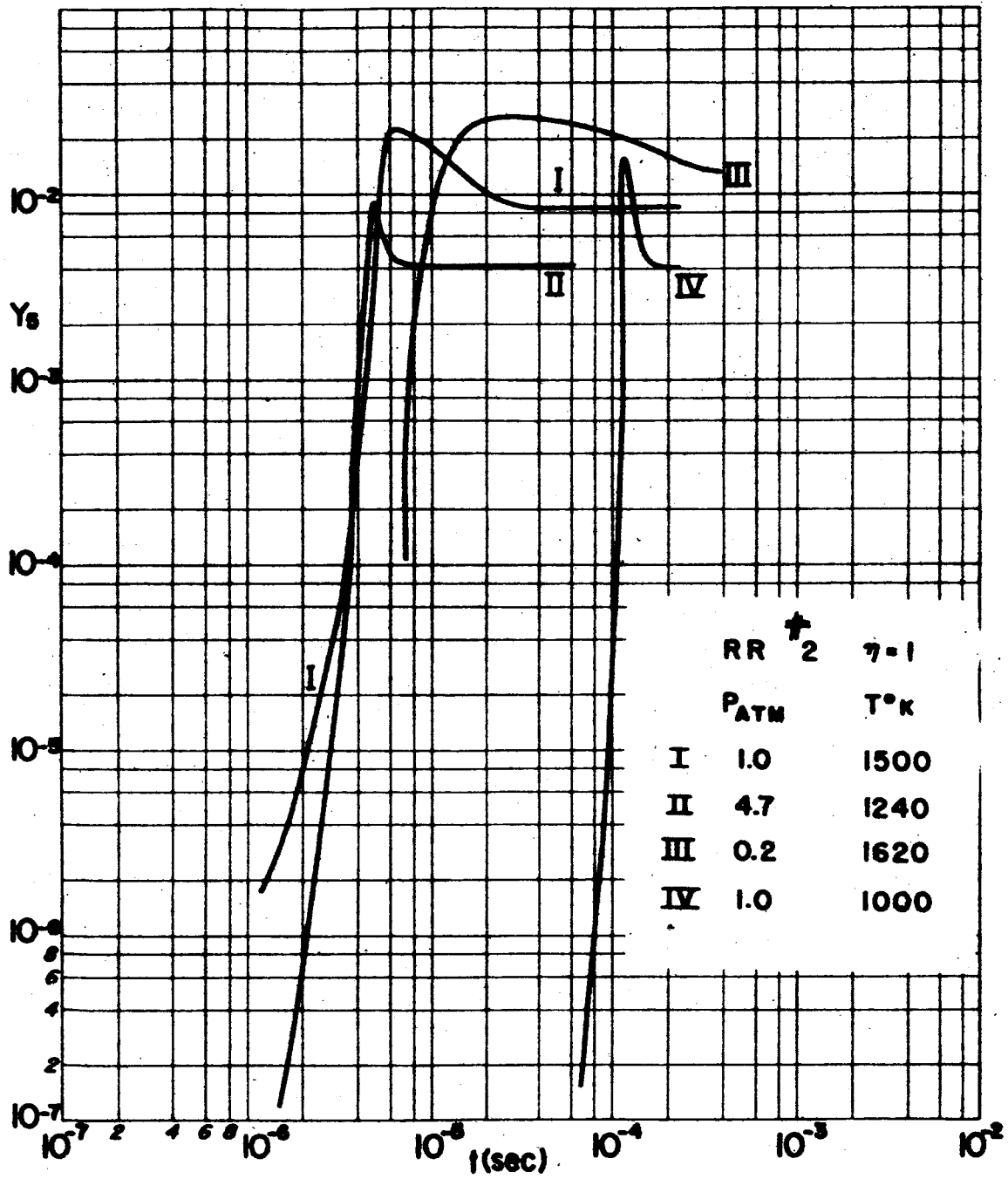


FIG. 16 Composition-Time Histories of Hydrogen-Air Mixtures at Constant Pressure.

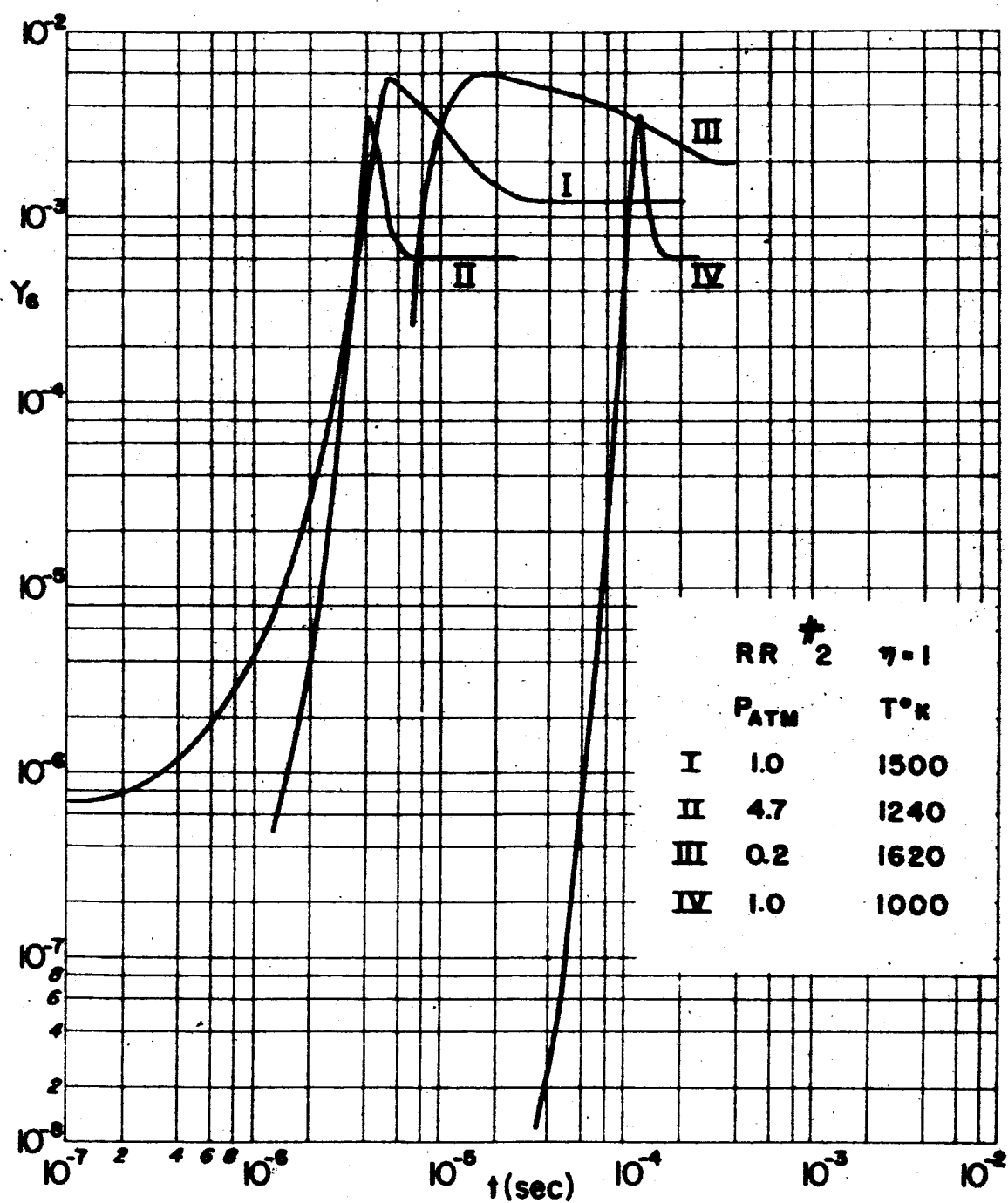


FIG. 1 Composition-Time Histories of Hydrogen-Air Mixtures at Constant Pressure.

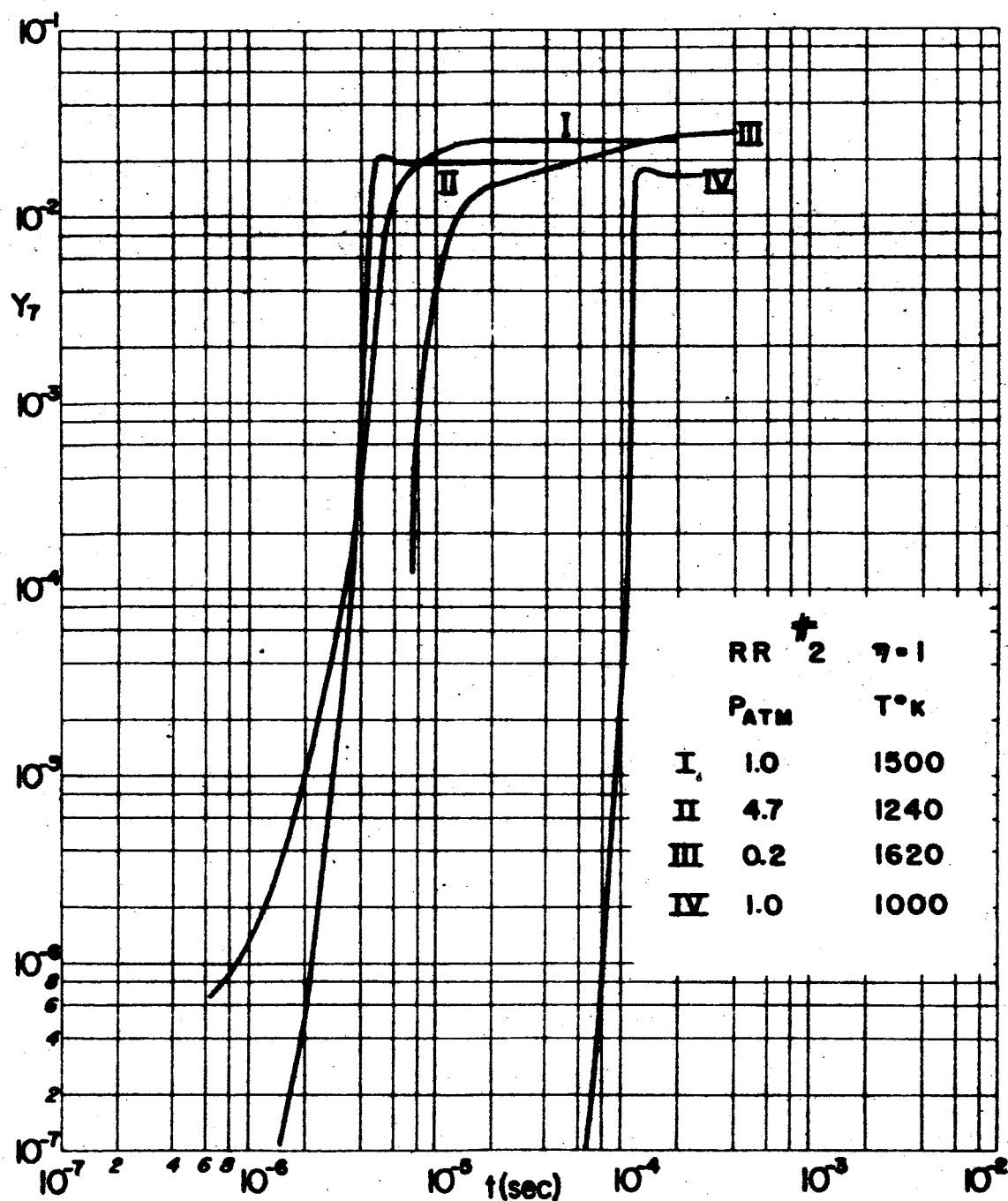
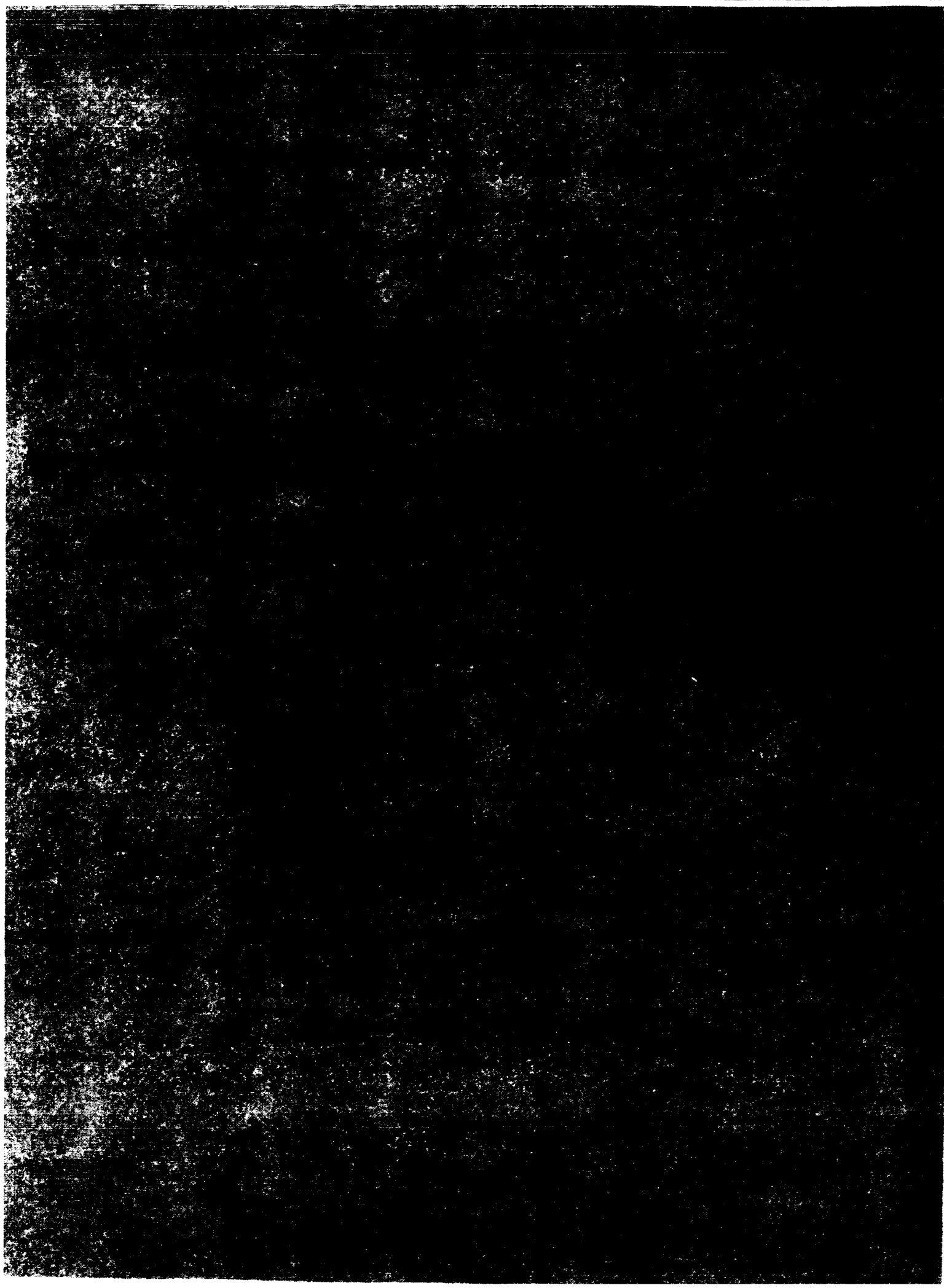
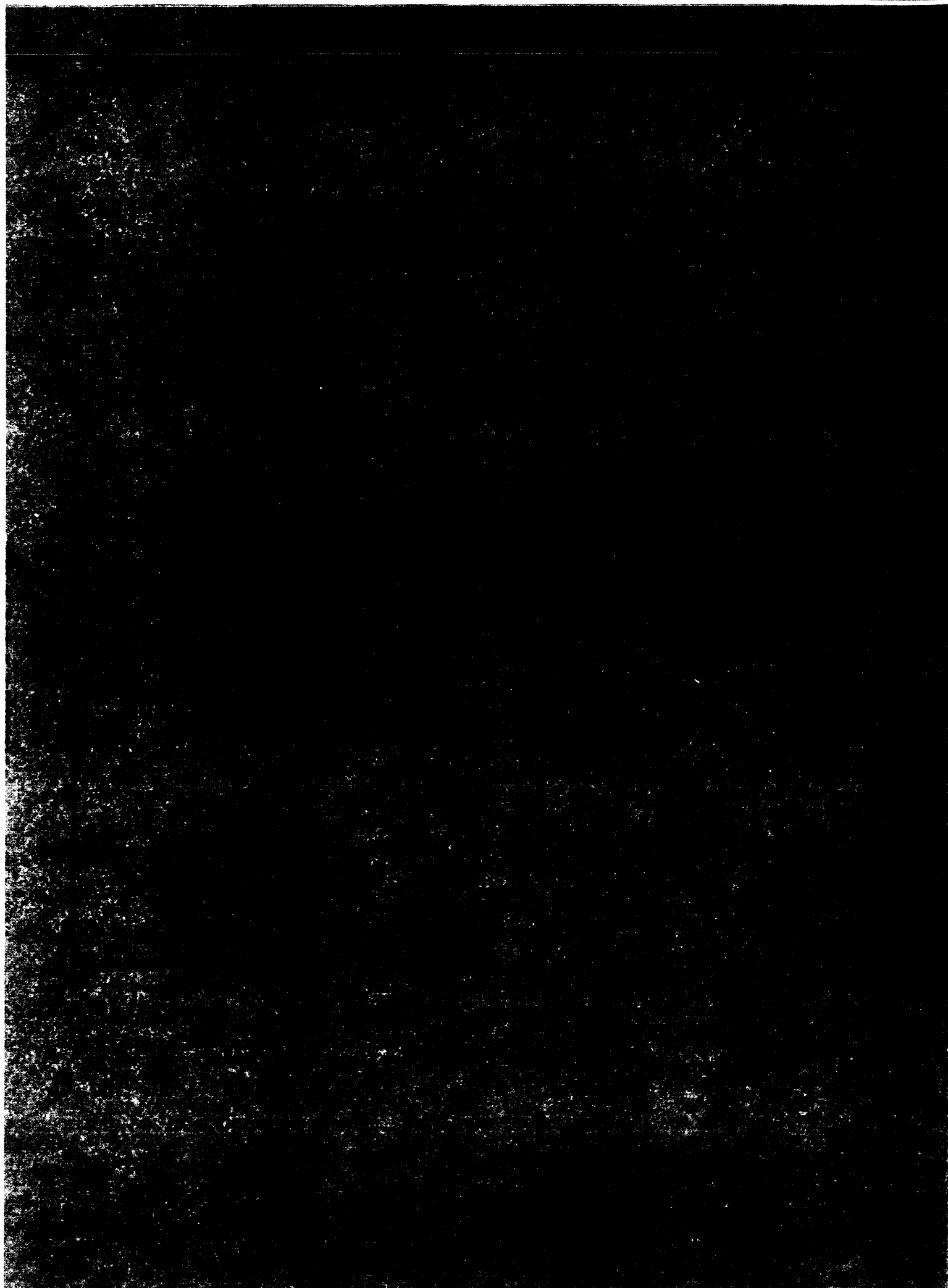


FIG. 11 Composition-Time Histories of Hydrogen-Air Mixtures at Constant Pressure.





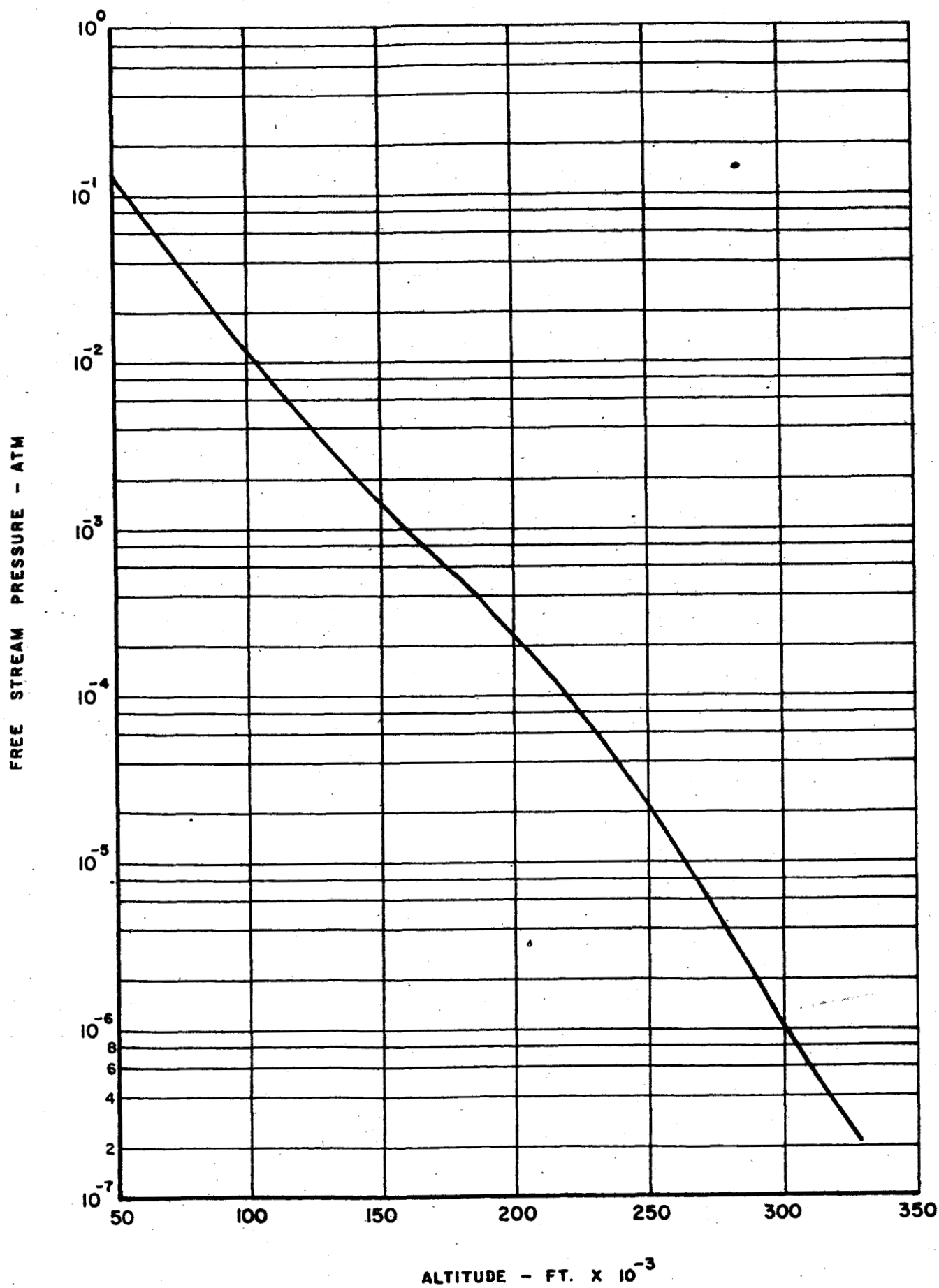


FIG. 4 AMBIENT PRESSURE VS. ALTITUDE

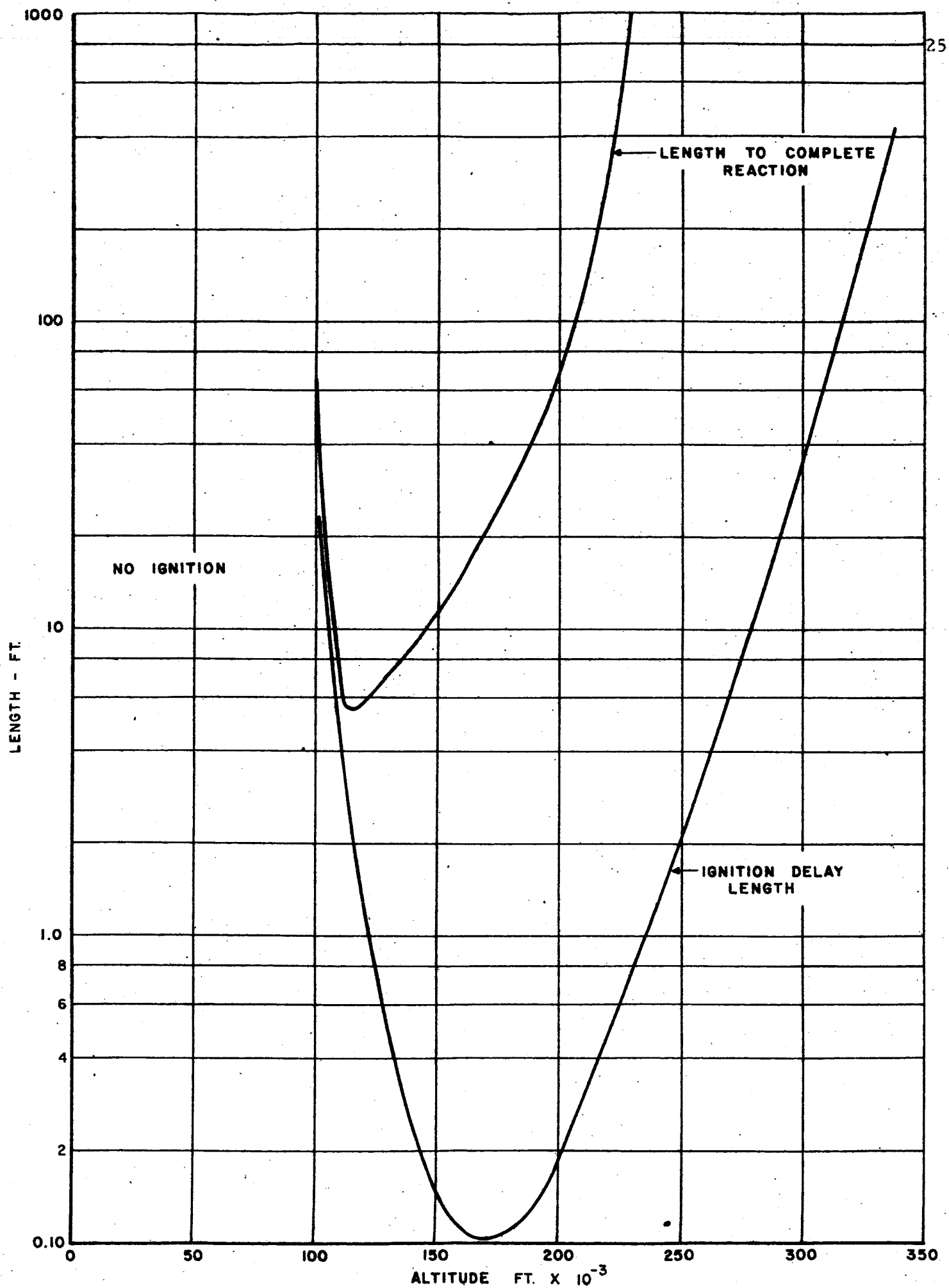


FIG. 5. CHEMICAL REACTION LENGTHS FOR NORMAL IGNITION OF HYDROGEN

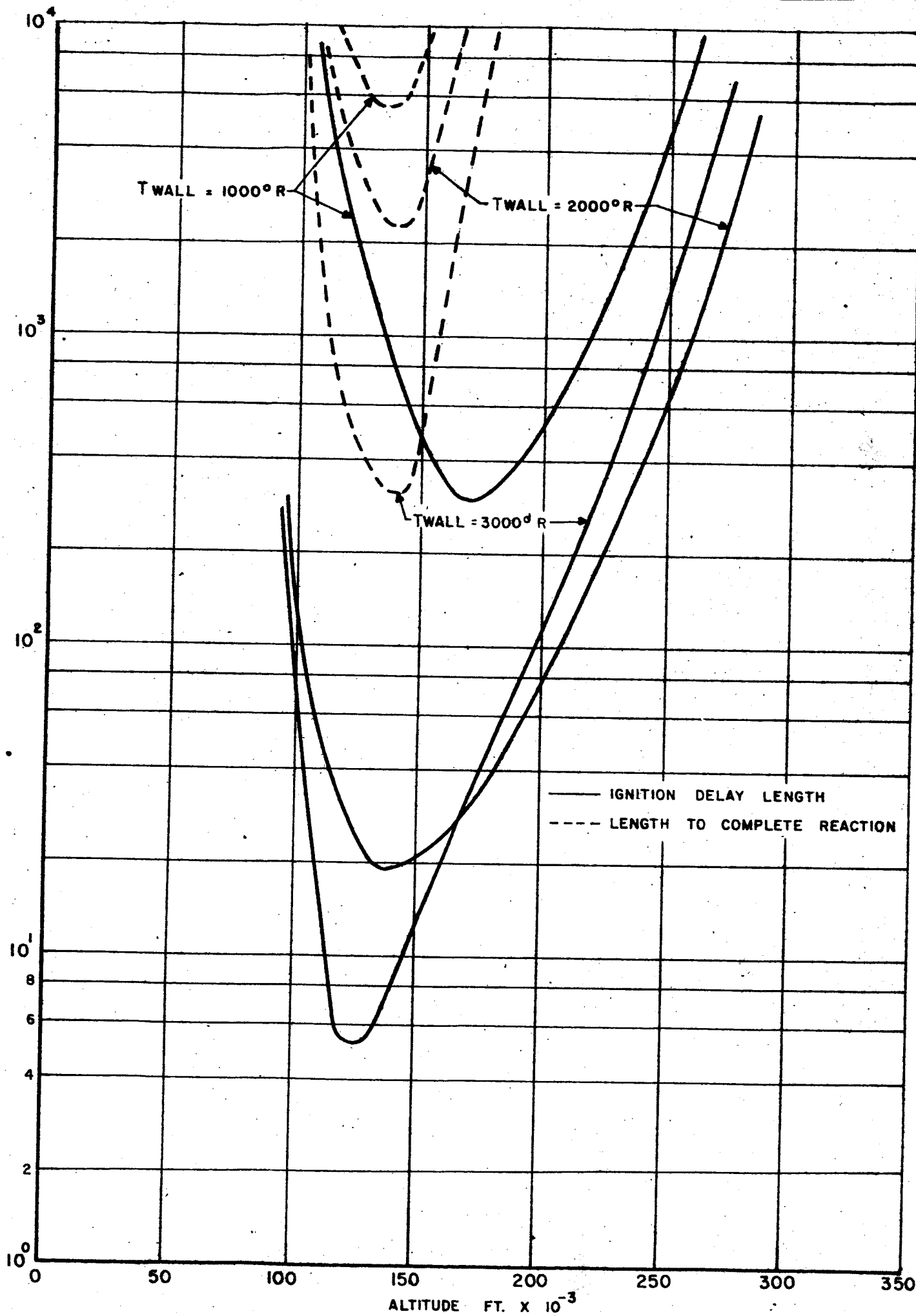


FIG. 6 CHEMICAL REACTION LENGTHS FOR INJECTION OF HYDROGEN THROUGH A TUBE

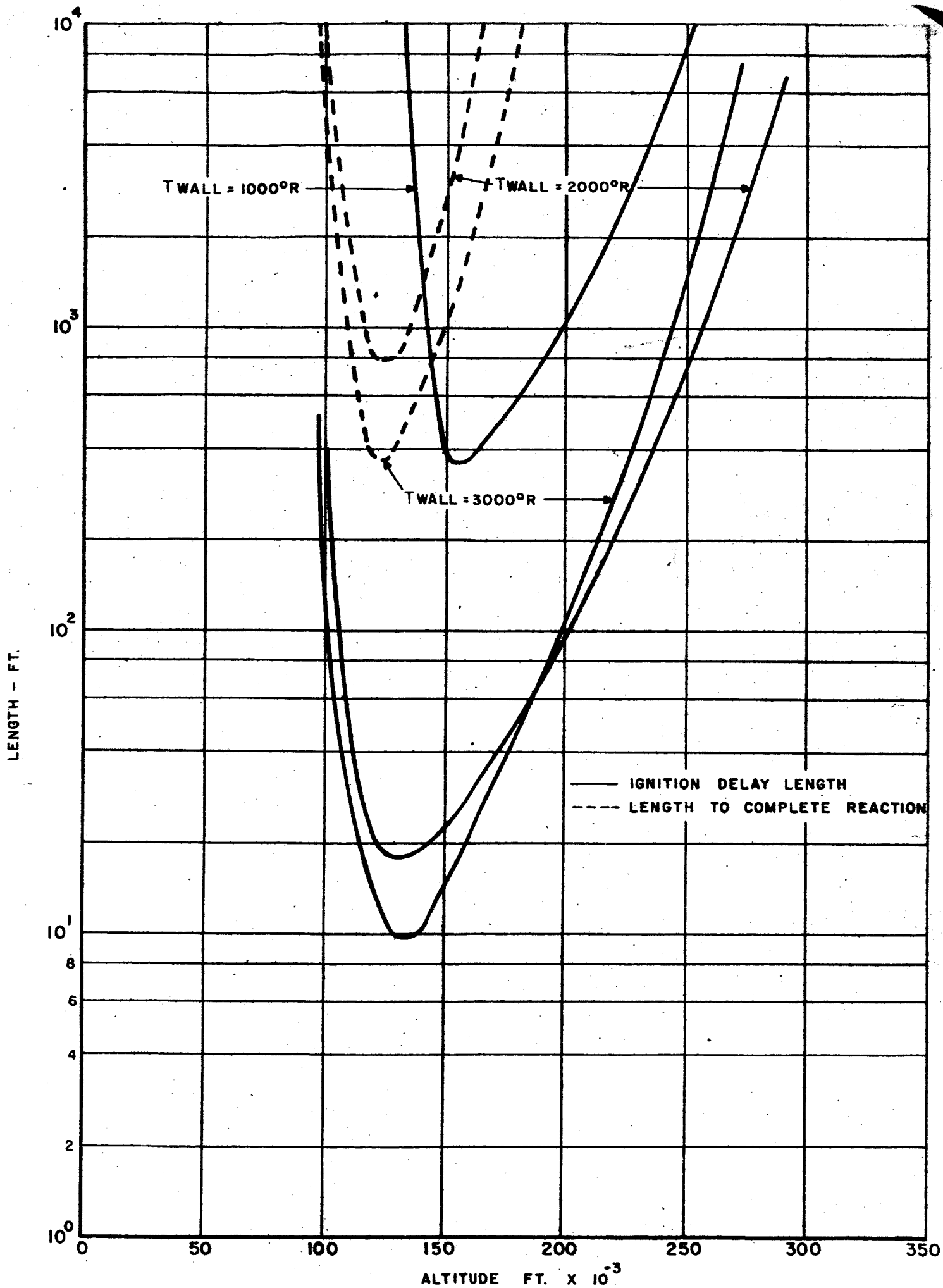


FIG. 7 CHEMICAL REACTION LENGTHS FOR SLOT INJECTION OF HYDROGEN